



Full wwPDB X-ray Structure Validation Report ⓘ

May 27, 2020 – 12:35 am BST

PDB ID : 2O1P
Title : Structure of yeast Poly(A) Polymerase in a somewhat closed state
Authors : Bohm, A.; Balbo, P.; Toth, J.
Deposited on : 2006-11-29
Resolution : 2.70 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

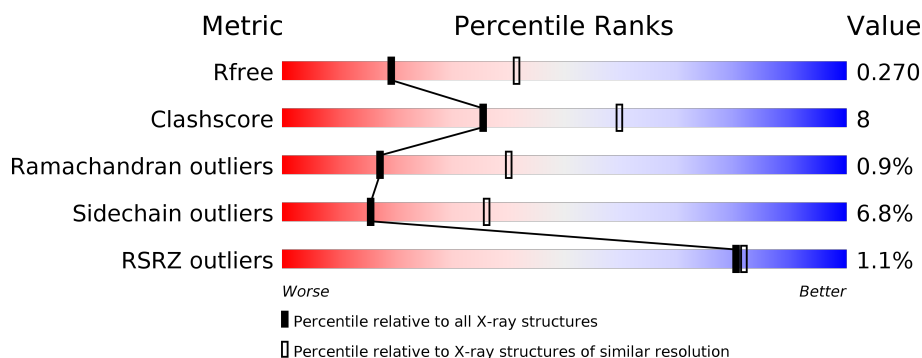
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	546	<div> <div>2%</div> <div> <div></div> <div>74%</div> <div>20%</div> <div>• •</div> </div> </div>
1	B	546	<div> <div>68%</div> <div>24%</div> <div>• •</div> </div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 8532 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Poly(A) polymerase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	523	Total	C	N	O	S	0	0	0
			4164	2680	704	764	16			
1	B	522	Total	C	N	O	S	0	0	0
			4185	2690	710	769	16			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	539	LEU	-	CLONING ARTIFACT	UNP P29468
A	540	GLU	-	CLONING ARTIFACT	UNP P29468
A	541	HIS	-	EXPRESSION TAG	UNP P29468
A	542	HIS	-	EXPRESSION TAG	UNP P29468
A	543	HIS	-	EXPRESSION TAG	UNP P29468
A	544	HIS	-	EXPRESSION TAG	UNP P29468
A	545	HIS	-	EXPRESSION TAG	UNP P29468
A	546	HIS	-	EXPRESSION TAG	UNP P29468
B	539	LEU	-	CLONING ARTIFACT	UNP P29468
B	540	GLU	-	CLONING ARTIFACT	UNP P29468
B	541	HIS	-	EXPRESSION TAG	UNP P29468
B	542	HIS	-	EXPRESSION TAG	UNP P29468
B	543	HIS	-	EXPRESSION TAG	UNP P29468
B	544	HIS	-	EXPRESSION TAG	UNP P29468
B	545	HIS	-	EXPRESSION TAG	UNP P29468
B	546	HIS	-	EXPRESSION TAG	UNP P29468

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	94	Total	O	0	0
			94	94		
2	B	89	Total	O	0	0
			89	89		

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Chain A:
-
- 74% 20%
- | Label | Value |
|-------|-------|
| NET | 29% |
| SER | 74% |
| SER | 74% |
| SER | 74% |
| Q4 | 20% |
| I9 | 74% |
| L25 | 74% |
| N26 | 74% |
| D27 | 74% |
| S28 | 74% |
| L29 | 74% |
| L55 | 74% |
| L58 | 74% |
| K69 | 74% |
| K70 | 74% |
| D74 | 74% |
| G75 | 74% |
| H76 | 74% |
| D79 | 74% |
| D100 | 74% |
| I101 | 74% |
| D102 | 74% |
| T103 | 74% |
| L104 | 74% |
| D121 | 74% |
| R125 | 74% |
| V136 | 74% |
| A139 | 74% |
| F140 | 74% |
| V141 | 74% |
| P142 | 74% |
| I143 | 74% |
| I144 | 74% |
| K145 | 74% |
| D154 | 74% |
| L155 | 74% |
| D161 | 74% |
| R178 | 74% |
| I179 | 74% |
| E182 | 74% |
| K183 | 74% |
| D184 | 74% |
| L185 | 74% |
| R186 | 74% |
| L187 | 74% |

- Chain B:
-
- 68% 24%
- | Position | Residue | Information Content (bits) |
|----------|---------|----------------------------|
| 1 | Y499 | 0.05 |
| 2 | G500 | 0.05 |
| 3 | D501 | 0.05 |
| 4 | V504 | 0.05 |
| 5 | F505 | 0.05 |
| 6 | N506 | 0.05 |
| 7 | D516 | 0.05 |
| 8 | V521 | 0.05 |
| 9 | F522 | 0.05 |
| 10 | D523 | 0.05 |
| 11 | K527 | 0.05 |
| 12 | R528 | 0.05 |
| 13 | P529 | 0.05 |
| 14 | SER | 0.05 |
| 15 | LYS | 0.05 |
| 16 | LYS | 0.05 |
| 17 | SER | 0.05 |
| 18 | LYS | 0.05 |
| 19 | ARG | 0.05 |
| 20 | LYS | 0.05 |
| 21 | ASN | 0.05 |
| 22 | LEU | 0.05 |
| 23 | LEU | 0.05 |
| 24 | GLU | 0.05 |
| 25 | HIS | 0.05 |
| 26 | HIS | 0.05 |
| 27 | HIS | 0.05 |
| 28 | HIS | 0.05 |
| 29 | HIS | 0.05 |
| 30 | HIS | 0.05 |
| 31 | D455 | 0.05 |
| 32 | A456 | 0.05 |
| 33 | P457 | 0.05 |
| 34 | K458 | 0.05 |
| 35 | S462 | 0.05 |
| 36 | T463 | 0.05 |
| 37 | K464 | 0.05 |
| 38 | Y465 | 0.05 |
| 39 | E473 | 0.05 |
| 40 | E477 | 0.05 |
| 41 | K478 | 0.05 |
| 42 | V479 | 0.05 |
| 43 | D480 | 0.05 |
| 44 | L491 | 0.05 |
| 45 | G492 | 0.05 |
| 46 | R493 | 0.05 |
| 47 | S494 | 0.05 |
| 48 | F495 | 0.05 |
| 49 | N496 | 0.05 |
| 50 | E497 | 0.05 |
| 51 | D498 | 0.05 |
| 52 | S152 | 0.05 |
| 53 | I153 | 0.05 |
| 54 | D154 | 0.05 |
| 55 | L155 | 0.05 |
| 56 | V165 | 0.05 |
| 57 | L169 | 0.05 |
| 58 | L176 | 0.05 |
| 59 | L177 | 0.05 |
| 60 | R178 | 0.05 |
| 61 | D181 | 0.05 |
| 62 | D184 | 0.05 |
| 63 | L188 | 0.05 |
| 64 | N189 | 0.05 |
| 65 | R192 | 0.05 |
| 66 | V193 | 0.05 |
| 67 | T194 | 0.05 |
| 68 | D195 | 0.05 |
| 69 | E196 | 0.05 |
| 70 | T214 | 0.05 |
| 71 | N226 | 0.05 |
| 72 | P230 | 0.05 |
| 73 | P231 | 0.05 |
| 74 | W236 | 0.05 |
| 75 | F356 | 0.05 |
| 76 | R357 | 0.05 |
| 77 | L359 | 0.05 |
| 78 | R342 | 0.05 |
| 79 | K359 | 0.05 |
| 80 | F360 | 0.05 |
| 81 | Y361 | 0.05 |
| 82 | L362 | 0.05 |
| 83 | E363 | 0.05 |
| 84 | I364 | 0.05 |
| 85 | T365 | 0.05 |
| 86 | H375 | 0.05 |
| 87 | L376 | 0.05 |
| 88 | K377 | 0.05 |
| 89 | K385 | 0.05 |
| 90 | L388 | 0.05 |
| 91 | L393 | 0.05 |
| 92 | P281 | 0.05 |
| 93 | L282 | 0.05 |
| 94 | D283 | 0.05 |
| 95 | V284 | 0.05 |
| 96 | R285 | 0.05 |
| 97 | V286 | 0.05 |
| 98 | W287 | 0.05 |
| 99 | K290 | 0.05 |
| 100 | A293 | 0.05 |

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	82.22Å 108.59Å 132.72Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	65.51 – 2.70 58.77 – 2.70	Depositor EDS
% Data completeness (in resolution range)	99.8 (65.51-2.70) 99.8 (58.77-2.70)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	0.10	Depositor
$\langle I/\sigma(I) \rangle$ ¹	6.22 (at 2.69Å)	Xtriage
Refinement program	REFMAC 5.2.0003	Depositor
R, R_{free}	0.195 , 0.275 0.193 , 0.270	Depositor DCC
R_{free} test set	1661 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å ²)	37.8	Xtriage
Anisotropy	0.243	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 40.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	8532	wwPDB-VP
Average B, all atoms (Å ²)	16.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.77% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.53	0/4258	0.81	22/5773 (0.4%)
1	B	0.53	0/4278	0.81	20/5794 (0.3%)
All	All	0.53	0/8536	0.81	42/11567 (0.4%)

There are no bond length outliers.

All (42) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	195	ASP	CB-CG-OD2	8.09	125.58	118.30
1	A	161	ASP	CB-CG-OD2	7.62	125.16	118.30
1	A	372	ASP	CB-CG-OD2	7.13	124.71	118.30
1	A	426	ASP	CB-CG-OD2	7.00	124.60	118.30
1	B	455	ASP	CB-CG-OD2	6.59	124.23	118.30
1	B	498	ASP	CB-CG-OD2	6.55	124.19	118.30
1	B	115	ASP	CB-CG-OD2	6.49	124.14	118.30
1	A	102	ASP	CB-CG-OD2	6.42	124.08	118.30
1	A	455	ASP	CB-CG-OD2	6.34	124.01	118.30
1	A	154	ASP	CB-CG-OD2	6.34	124.01	118.30
1	B	529	PRO	N-CA-CB	6.31	110.87	103.30
1	A	337	ASP	CB-CG-OD2	6.28	123.95	118.30
1	A	121	ASP	CB-CG-OD2	6.20	123.88	118.30
1	A	79	ASP	CB-CG-OD2	6.19	123.88	118.30
1	A	295	ASP	CB-CG-OD2	6.18	123.86	118.30
1	B	516	ASP	CB-CG-OD2	6.12	123.81	118.30
1	B	121	ASP	CB-CG-OD2	6.11	123.80	118.30
1	A	516	ASP	CB-CG-OD2	6.02	123.72	118.30
1	A	420	ASP	CB-CG-OD2	6.00	123.70	118.30
1	B	102	ASP	CB-CG-OD2	5.95	123.65	118.30
1	B	523	ASP	CB-CG-OD2	5.94	123.65	118.30
1	B	445	ASP	CB-CG-OD2	5.93	123.64	118.30
1	B	195	ASP	CB-CG-OD2	5.91	123.62	118.30
1	A	442	LEU	CA-CB-CG	5.87	128.80	115.30
1	B	74	ASP	CB-CG-OD2	5.80	123.52	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	295	ASP	CB-CG-OD2	5.77	123.50	118.30
1	A	469	ASP	CB-CG-OD2	5.75	123.47	118.30
1	A	100	ASP	CB-CG-OD2	5.71	123.44	118.30
1	B	501	ASP	CB-CG-OD2	5.56	123.30	118.30
1	B	419	ASP	CB-CG-OD2	5.50	123.25	118.30
1	B	480	ASP	CB-CG-OD2	5.48	123.24	118.30
1	B	173	ASP	CB-CG-OD2	5.48	123.23	118.30
1	A	74	ASP	CB-CG-OD2	5.42	123.18	118.30
1	A	279	ASP	CB-CG-OD2	5.39	123.15	118.30
1	B	181	ASP	CB-CG-OD2	5.37	123.13	118.30
1	B	138	ASP	CB-CG-OD2	5.34	123.11	118.30
1	B	125	ARG	NE-CZ-NH2	-5.22	117.69	120.30
1	A	184	ASP	CB-CG-OD2	5.22	123.00	118.30
1	A	27	ASP	CB-CG-OD2	5.18	122.96	118.30
1	B	184	ASP	CB-CG-OD2	5.13	122.92	118.30
1	A	523	ASP	CB-CG-OD2	5.13	122.92	118.30
1	A	501	ASP	CB-CG-OD2	5.00	122.80	118.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4164	0	4157	62	0
1	B	4185	0	4198	74	0
2	A	94	0	0	3	0
2	B	89	0	0	4	0
All	All	8532	0	8355	135	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 8.

All (135) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:483:ILE:HG13	1:A:484:PRO:HD3	1.18	1.13
1:B:365:THR:HG23	1:B:463:THR:HG22	1.42	1.00
1:A:456:ALA:HB3	1:A:457:PRO:HD3	1.49	0.92
1:A:227:ILE:H	1:A:227:ILE:HD12	1.34	0.91
1:A:326:GLN:HE22	1:A:357:ARG:HH22	1.28	0.78
1:B:428:TYR:OH	1:B:463:THR:HG21	1.83	0.78
1:A:26:ASN:HD22	1:A:253:ALA:H	1.32	0.76
1:B:26:ASN:HD22	1:B:253:ALA:H	1.35	0.74
1:A:483:ILE:CG1	1:A:484:PRO:HD3	2.11	0.71
1:A:26:ASN:HD21	1:A:252:SER:HB2	1.54	0.70
1:A:314:HIS:HB3	2:A:603:HOH:O	1.93	0.68
1:A:430:SER:O	1:A:434:GLU:HB2	1.94	0.67
1:A:369:ARG:HB2	1:A:504:VAL:HA	1.77	0.67
1:A:443:VAL:HG21	1:A:458:LYS:HE3	1.77	0.66
1:B:326:GLN:HE22	1:B:357:ARG:HH22	1.44	0.65
1:B:363:GLU:HG3	1:B:465:TYR:CE2	2.34	0.63
1:B:455:ASP:HA	2:B:618:HOH:O	1.98	0.63
1:A:456:ALA:CB	1:A:457:PRO:HD3	2.25	0.62
1:B:447:ASN:OD1	1:B:448:LYS:N	2.30	0.62
1:A:293:ALA:HA	1:A:296:ARG:HG3	1.80	0.62
1:A:528:ARG:O	1:A:528:ARG:HG2	2.01	0.59
1:A:227:ILE:H	1:A:227:ILE:CD1	2.07	0.59
1:B:125:ARG:HA	1:B:130:LEU:HD12	1.85	0.58
1:B:385:LYS:HA	1:B:388:LEU:HD13	1.86	0.58
1:B:359:LYS:HB2	1:B:360:PHE:CD1	2.39	0.58
1:B:293:ALA:HA	1:B:296:ARG:HE	1.68	0.58
1:B:264:SER:HB3	1:B:328:PHE:HB3	1.86	0.57
1:A:26:ASN:ND2	1:A:253:ALA:H	2.02	0.57
1:A:368:THR:OG1	1:A:375:HIS:HD2	1.88	0.56
1:A:439:ALA:HA	1:B:290:LYS:O	2.04	0.56
1:B:388:LEU:HD12	1:B:388:LEU:N	2.20	0.56
1:A:409:PHE:HA	2:A:563:HOH:O	2.05	0.55
1:A:357:ARG:HB2	2:A:611:HOH:O	2.06	0.55
1:B:326:GLN:HE22	1:B:357:ARG:NH2	2.05	0.54
1:A:136:VAL:HG12	1:A:139:ALA:HB2	1.89	0.54
1:B:26:ASN:ND2	1:B:253:ALA:H	2.03	0.54
1:B:226:ASN:HA	1:B:230:PHE:O	2.08	0.54
1:A:424:ILE:HA	1:A:437:LEU:HD21	1.91	0.53
1:A:483:ILE:HG13	1:A:484:PRO:CD	2.12	0.53
1:A:528:ARG:CG	1:A:528:ARG:O	2.57	0.53
1:B:153:ILE:HG22	1:B:155:LEU:HG	1.91	0.53
1:A:281:PRO:O	1:A:284:VAL:CG1	2.57	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:326:GLN:NE2	1:A:357:ARG:HH22	2.03	0.52
1:A:140:PHE:CD2	1:A:141:VAL:HG23	2.44	0.52
1:A:143:ILE:HD11	1:A:154:ASP:HB3	1.91	0.52
1:B:75:GLY:HA2	1:B:78:ARG:CZ	2.40	0.52
1:B:388:LEU:H	1:B:388:LEU:HD12	1.74	0.52
1:B:495:PHE:HA	2:B:622:HOH:O	2.10	0.51
1:A:145:LYS:HG2	1:A:154:ASP:OD1	2.10	0.51
1:B:493:ARG:HH21	1:B:506:ASN:HA	1.76	0.51
1:B:446:GLU:HG2	1:B:447:ASN:N	2.26	0.51
1:A:281:PRO:O	1:A:284:VAL:HG13	2.11	0.51
1:A:142:PRO:HG2	1:A:183:LYS:HD3	1.92	0.51
1:B:286:VAL:HG12	1:B:287:TRP:H	1.75	0.50
1:B:286:VAL:HG12	1:B:287:TRP:N	2.26	0.50
1:B:165:VAL:HG13	1:B:169:LEU:HD22	1.92	0.50
1:A:217:TRP:O	1:A:221:ARG:HG2	2.12	0.49
1:A:474:ASN:C	1:A:476:LYS:H	2.15	0.49
1:A:182:GLU:HG3	1:A:186:ARG:CZ	2.42	0.49
1:B:192:ARG:O	1:B:196:GLU:HG3	2.12	0.49
1:B:364:ILE:O	1:B:463:THR:HA	2.12	0.49
1:B:56:GLN:HE22	1:B:83:LYS:HA	1.78	0.49
1:B:428:TYR:CZ	1:B:463:THR:HG21	2.47	0.49
1:B:26:ASN:HD22	1:B:253:ALA:N	2.06	0.48
1:B:417:THR:HB	1:B:420:ASP:H	1.79	0.48
1:A:495:PHE:O	1:A:496:ASN:CB	2.61	0.47
1:B:40:GLU:HG2	2:B:628:HOH:O	2.14	0.47
1:B:3:SER:OG	1:B:4:GLN:N	2.47	0.47
1:B:75:GLY:HA2	1:B:78:ARG:NH2	2.30	0.47
1:B:473:GLU:OE1	1:B:479:VAL:HG13	2.15	0.47
1:B:355:PHE:CG	1:B:521:VAL:HG13	2.50	0.47
1:B:110:HIS:H	1:B:110:HIS:CD2	2.32	0.47
1:A:178:ARG:O	1:A:179:ASN:HB2	2.13	0.46
1:B:456:ALA:O	1:B:458:LYS:HD2	2.14	0.46
1:A:388:LEU:HA	1:A:391:MET:HE3	1.97	0.46
1:B:496:ASN:HB3	1:B:499:TYR:H	1.80	0.46
1:B:175:ASN:C	1:B:177:LEU:H	2.19	0.46
1:B:26:ASN:HD21	1:B:252:SER:HB2	1.80	0.46
1:B:73:SER:HB2	1:B:76:MET:H	1.81	0.45
1:B:178:ARG:HB2	1:B:178:ARG:NH1	2.32	0.45
1:A:104:LEU:HD21	1:A:188:LEU:HD12	1.99	0.45
1:A:282:LEU:O	1:A:284:VAL:HG22	2.17	0.45
1:A:364:ILE:O	1:A:463:THR:HA	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:283:GLN:O	1:A:284:VAL:O	2.35	0.44
1:A:444:THR:HG23	1:A:445:ASP:N	2.32	0.44
1:B:358:TYR:HB2	1:B:361:TYR:CZ	2.53	0.44
1:A:226:ASN:HA	1:A:230:PHE:O	2.16	0.44
1:B:416:PRO:HA	1:B:457:PRO:HG2	1.99	0.44
1:B:342:LYS:HD2	2:B:608:HOH:O	2.17	0.44
1:A:445:ASP:HA	1:A:446:GLU:HA	1.72	0.44
1:B:407:LYS:HA	1:B:408:PRO:HD2	1.89	0.44
1:B:277:ILE:CG2	1:B:286:VAL:HG11	2.47	0.44
1:B:430:SER:O	1:B:434:GLU:HB2	2.17	0.44
1:A:363:GLU:HB3	1:A:510:ARG:HB3	1.99	0.44
1:B:427:LYS:HD3	1:B:433:THR:HB	2.00	0.43
1:A:375:HIS:CG	1:A:460:TYR:HB3	2.53	0.43
1:B:51:VAL:HG21	1:B:151:ILE:HD12	1.99	0.43
1:A:25:LEU:HD22	1:A:338:ILE:HG22	2.00	0.43
1:B:491:LEU:O	1:B:495:PHE:HB2	2.19	0.43
1:A:453:ILE:O	1:A:454:LYS:HE3	2.18	0.43
1:A:481:ILE:O	1:A:484:PRO:HD2	2.18	0.43
1:B:347:ASN:O	1:B:350:GLU:HB2	2.18	0.43
1:B:501:ASP:HB3	1:B:504:VAL:HG22	2.00	0.43
1:B:189:ASN:O	1:B:193:VAL:HG23	2.19	0.43
1:B:375:HIS:HE1	1:B:462:SER:OG	2.00	0.43
1:B:131:ASP:HB2	1:B:147:LYS:HB3	2.00	0.43
1:A:224:TYR:O	1:A:225:ALA:HB2	2.19	0.43
1:B:415:CYS:HA	1:B:416:PRO:HD3	1.69	0.43
1:A:495:PHE:O	1:A:496:ASN:HB3	2.20	0.42
1:A:284:VAL:HG21	1:A:307:TYR:OH	2.20	0.42
1:B:307:TYR:HA	1:B:308:PRO:HA	1.84	0.42
1:B:428:TYR:CE2	1:B:463:THR:HG21	2.55	0.42
1:B:398:GLY:HA3	1:B:479:VAL:HG11	2.02	0.42
1:A:121:ASP:O	1:A:125:ARG:HG3	2.20	0.42
1:A:140:PHE:O	1:A:142:PRO:HD3	2.20	0.41
1:B:300:MET:SD	1:B:321:LYS:HG3	2.61	0.41
1:B:496:ASN:HB3	1:B:498:ASP:N	2.35	0.41
1:A:121:ASP:OD2	1:A:125:ARG:HD2	2.21	0.41
1:A:55:LEU:HD23	1:A:58:LEU:HD12	2.02	0.41
1:A:456:ALA:CB	1:A:457:PRO:CD	2.96	0.41
1:A:9:ILE:HG22	1:A:276:PRO:HD3	2.03	0.41
1:B:86:THR:O	1:B:91:ARG:HD3	2.21	0.41
1:A:307:TYR:HA	1:A:308:PRO:HA	1.90	0.41
1:A:407:LYS:HE3	1:A:407:LYS:HB2	1.93	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:141:VAL:HA	1:B:142:PRO:HD3	1.85	0.41
1:A:284:VAL:HG11	1:A:307:TYR:OH	2.21	0.41
1:B:527:LYS:HD3	1:B:527:LYS:HA	1.71	0.41
1:B:231:PRO:HG2	1:B:236:TRP:CZ2	2.56	0.40
1:B:13:VAL:HG23	1:B:246:LEU:HD22	2.03	0.40
1:A:415:CYS:HB3	1:A:416:PRO:O	2.21	0.40
1:B:270:GLN:HG3	1:B:271:PRO:HD2	2.02	0.40
1:B:477:GLU:CD	1:B:477:GLU:H	2.25	0.40
1:B:313:THR:HB	1:B:316:ILE:HD12	2.03	0.40
1:B:178:ARG:HB2	1:B:178:ARG:CZ	2.52	0.40
1:B:415:CYS:HB2	1:B:420:ASP:HB3	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	519/546 (95%)	486 (94%)	27 (5%)	6 (1%)	13	32
1	B	518/546 (95%)	493 (95%)	22 (4%)	3 (1%)	25	50
All	All	1037/1092 (95%)	979 (94%)	49 (5%)	9 (1%)	17	40

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	284	VAL
1	A	456	ALA
1	B	282	LEU
1	A	225	ALA
1	A	496	ASN
1	A	520	GLU
1	B	281	PRO

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Mol	Chain	Res	Type
1	B	71	ASN
1	A	416	PRO

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	453/488 (93%)	429 (95%)	24 (5%)	22	48
1	B	459/488 (94%)	421 (92%)	38 (8%)	11	25
All	All	912/976 (93%)	850 (93%)	62 (7%)	16	36

All (62) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	GLN
1	A	29	LEU
1	A	69	LYS
1	A	70	LYS
1	A	76	MET
1	A	155	LEU
1	A	227	ILE
1	A	239	LEU
1	A	278	GLU
1	A	285	ARG
1	A	341	ASN
1	A	377	LYS
1	A	381	LEU
1	A	387	ARG
1	A	393	LEU
1	A	415	CYS
1	A	419	ASP
1	A	453	ILE
1	A	454	LYS
1	A	462	SER
1	A	476	LYS

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Mol	Chain	Res	Type
1	A	491	LEU
1	A	526	GLU
1	A	528	ARG
1	B	4	GLN
1	B	42	GLU
1	B	61	ARG
1	B	68	LYS
1	B	73	SER
1	B	74	ASP
1	B	79	ASP
1	B	121	ASP
1	B	130	LEU
1	B	136	VAL
1	B	172	SER
1	B	188	LEU
1	B	214	ILE
1	B	239	LEU
1	B	242	ARG
1	B	262	ILE
1	B	284	VAL
1	B	285	ARG
1	B	310	MET
1	B	340	SER
1	B	357	ARG
1	B	376	LEU
1	B	377	LYS
1	B	393	LEU
1	B	407	LYS
1	B	410	GLU
1	B	417	THR
1	B	423	MET
1	B	441	LYS
1	B	446	GLU
1	B	455	ASP
1	B	464	MET
1	B	477	GLU
1	B	479	VAL
1	B	493	ARG
1	B	494	SER
1	B	496	ASN
1	B	527	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such

sidechains are listed below:

Mol	Chain	Res	Type
1	A	26	ASN
1	A	50	GLN
1	A	56	GLN
1	A	60	GLN
1	A	162	GLN
1	A	179	ASN
1	A	326	GLN
1	A	336	ASN
1	A	375	HIS
1	A	438	ASN
1	A	490	ASN
1	A	496	ASN
1	B	4	GLN
1	B	26	ASN
1	B	56	GLN
1	B	60	GLN
1	B	110	HIS
1	B	288	ASN
1	B	326	GLN
1	B	336	ASN
1	B	375	HIS
1	B	425	GLN
1	B	490	ASN
1	B	506	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	523/546 (95%)	-0.06	11 (2%) 63 65	2, 13, 36, 52	0
1	B	522/546 (95%)	-0.20	1 (0%) 95 96	4, 15, 34, 39	0
All	All	1045/1092 (95%)	-0.13	12 (1%) 80 82	2, 14, 36, 52	0

All (12) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	413	TYR	6.0
1	A	282	LEU	3.6
1	A	532	LYS	3.4
1	B	529	PRO	3.1
1	A	529	PRO	2.7
1	A	456	ALA	2.7
1	A	457	PRO	2.5
1	A	419	ASP	2.4
1	A	281	PRO	2.4
1	A	475	LYS	2.1
1	A	430	SER	2.0
1	A	479	VAL	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.